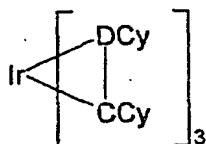


What is claimed is:

1. A process for preparing homoleptic Ir(III) complexes of the formula (I)

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formula (I)

in which:

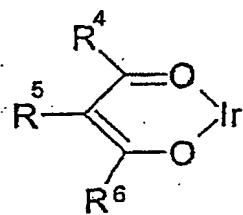
- 10 CyD is a cyclic group which contains at least one donor atom via which the cyclic group is bonded to the metal and which may in turn bear one or more substituents R; the CyD and CyC groups are joined together via a covalent bond;
- 15 CyC is a cyclic group which contains a carbon atom via which the cyclic group is bonded to the metal and which may in turn bear one or more substituents R;
- 20 R is the same or different at each instance and is H, F, Cl, Br, I, NO<sub>2</sub>, CN, a straight-chain or branched or cyclic alkyl or alkoxy group having from 1 to 20 carbon atoms, in which one or more nonadjacent CH<sub>2</sub> groups may be replaced by -O-, -S-, -NR<sup>1</sup>-, -CONR<sup>2</sup>-, -CO-O-, -CR<sup>1</sup>=CR<sup>1</sup>- or -C≡C-, and in which one or more hydrogen atoms may be replaced by F, or an aryl or heteroaryl group which has from 4 to 25 carbon atoms and may be substituted by one or more nonaromatic R radicals; where a plurality of substituents R, both on the same ring and on the two different rings, together may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system;
- 30
- 35

R<sup>1</sup> and R<sup>2</sup> are the same or different at each instance and are H or an aliphatic or aromatic hydrocarbon radical having from 1 to 20 carbon atoms,

5

characterized by the reaction of an iridium(III)-containing reactant which contains at least one diketonate structural unit of the formula (II)

10



formula (II)

in which:

R<sup>4</sup>, R<sup>6</sup> are the same or different at each instance and are a linear, branched or cyclic alkyl group having 1-20 carbon atoms, in which one or more nonadjacent CH<sub>2</sub> groups may be replaced by -O-, -S-, -NR<sup>1</sup>-, -CONR<sup>2</sup>-, -CO-O-, -CR<sup>1</sup>=CR<sup>1</sup>- or -C≡C-, and in which one or more hydrogen atoms may be replaced by F or aromatic groups each having from 3 to 14 carbon atoms, or an aryl and/or heteroaryl group having 3-20 carbon atoms or an alkoxy group OR<sup>1</sup>,

R<sup>5</sup> is the same or different at each instance and is a linear or branched alkyl group having 1-20 carbon atoms, in which one or more nonadjacent CH<sub>2</sub> groups may be replaced by -O-, -S-, -NR<sup>1</sup>-, -CONR<sup>2</sup>-, -CO-O-, -CR<sup>1</sup>=CR<sup>1</sup>- or -C≡C-, and in which one or more hydrogen atoms may be replaced by F or aromatic groups each having from 3 to 14 carbon atoms, or an aryl and/or heteroaryl group having 3-20 carbon atoms,

R<sup>1</sup> and R<sup>2</sup> are the same or different at each instance and are H or an aliphatic or aromatic hydrocarbon radical having from 1 to 20 carbon atoms,

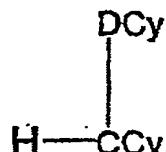
5 excluding homoleptic diketonate complexes of the formula (II) and compounds of the formula (II) which contain two ligands of the formula (III)



10 formula (III)

where the symbols CyC and CyD in formula (III) are each as defined under formula (I),

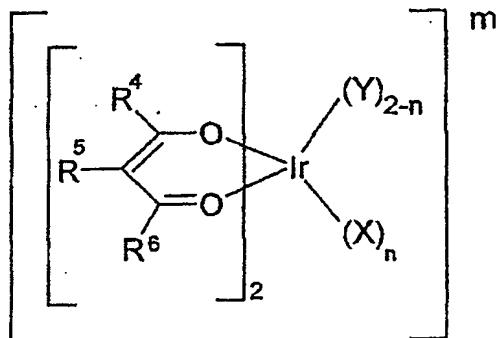
15 with a compound of the formula (IV)



formula (IV)

20 in which the symbols CyD and CyC are each as defined under formula (I).

25 2. The process as claimed in claim 1, characterized in that the iridium(III)-containing reactant contains a structure of the formula (V)



formula (V)

where the symbols  $R^4$ ,  $R^5$  and  $R^6$  are each as defined in  
5 claim 1,

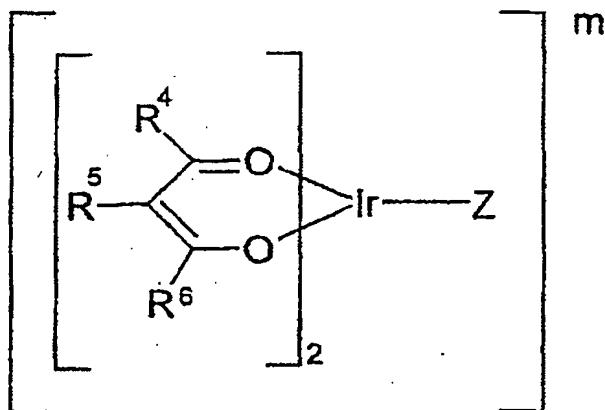
$X$  is the same or different at each instance and  
is a monovalent anion,

$Y$  is the same or different at each instance and  
is an uncharged monodentate ligand,

10  $n$  is 0, 1 or 2 and

$m$  is 1- when  $n = 2$ , is 0 when  $n = 1$  or is 1+  
when  $n = 0$ .

3. The process as claimed in claim 1, characterized  
15 in that the iridium(III)-containing reactant contains a  
structure of the formula (VI)



formula (VI)

where  $R^4$ ,  $R^5$  and  $R^6$  are each as defined in claim 1 and where

$Z$  is the same or different at each instance and is

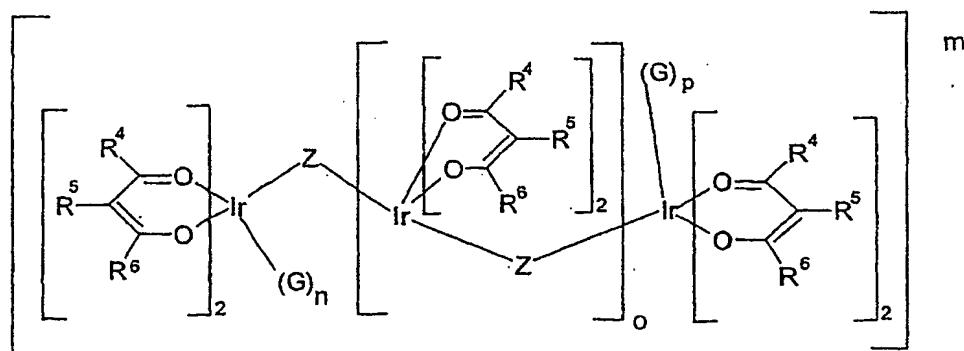
5 and uncharged bidentate and/or bridging ligand  $Z^0$ ,

a monoanionic bidentate and/or bridging ligand  $Z^1$

or a dianionic bidentate and/or bridging 10 ligand  $Z^2$ , and

m is 1+ when  $Z = Z^0$ , is 0 when  $Z = Z^1$  and is 1- when  $Z = Z^2$ .

4. The process as claimed in claim 1, characterized 15 in that the iridium(III)-containing reactant contains a structure of the formula (VII)



formula (VII)

20

where  $R^4$ ,  $R^5$ ,  $R^6$  and  $Z$  are each as defined in claim 1 and claim 3,

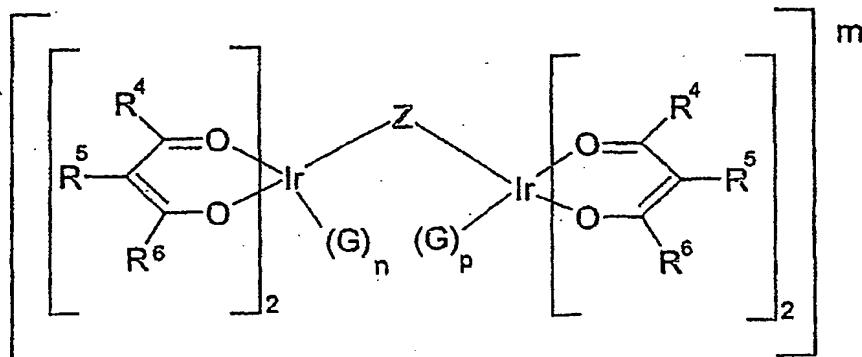
G is the same or different at each instance and is either a monovalent anion X or an uncharged monodentate ligand Y,

25 n, p are the same or different at each instance and are 0 or 1,

o can assume integer values from 0 to 100 000 and

30 m may be from  $(o+2)+$  to  $(o+2)-$ .

5. The process as claimed in claim 1, characterized in that the iridium(III)-containing reactant contains a structure of the formula (VIII)



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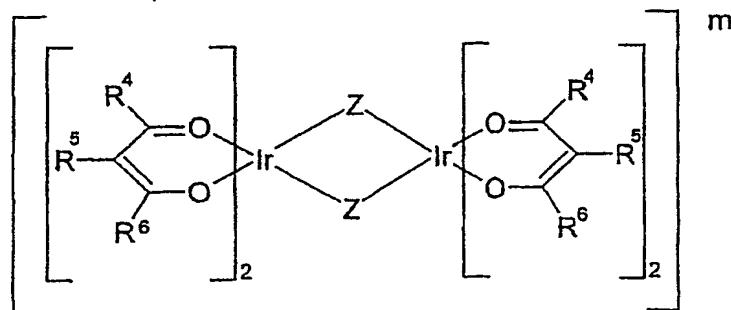
formula (VIII)

where the symbols and indices R<sup>4</sup>, R<sup>5</sup>, R<sup>6</sup>, G, Z, n and p are each as defined in claim 1, 3 and 4 and in which

10 m is 2+, 1+, 0, 1- or 2-.

6. The process as claimed in claim 1, characterized in that the iridium(III)-containing reactant contains a structure of the formula (IX)

15



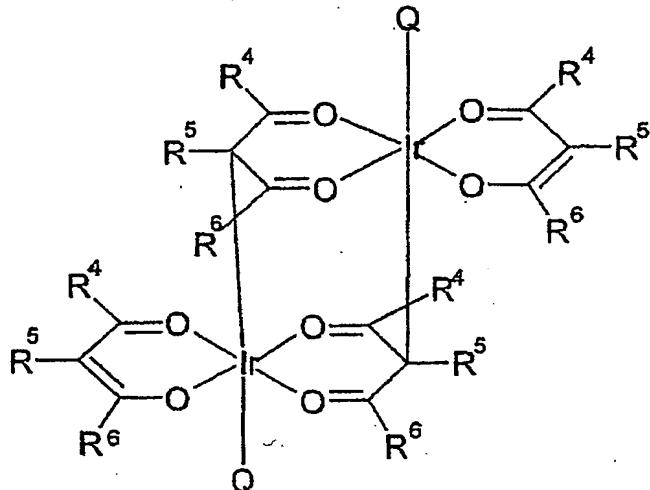
formula (IX)

where the symbols R<sup>1</sup>, R<sup>2</sup>, R<sup>4</sup>, R<sup>5</sup>, R<sup>6</sup> and Z are each as

20 defined in claim 1 and claim 3 and in which

m is 2+, 1+, 0, 1- or 2-.

7. The process as claimed in claim 1, characterized in that the iridium(III)-containing reactant contains a structure of the formula (X)



5

formula (X)

where the symbols R<sup>4</sup>, R<sup>5</sup> and R<sup>6</sup> are each as defined in claim 1 and where

10 Q is the same or different at each instance and is a monovalent anion.

8. The process as claimed in one or more of claims 2, 4 and 5, characterized in that the iridium(III)-containing reactant contains a compound of the formula (V), (VII) and/or (VIII) and X is the same or different at each instance and is OH<sup>-</sup>, F<sup>-</sup>, Cl<sup>-</sup>, Br<sup>-</sup>, I<sup>-</sup>, SCN<sup>-</sup>, CN<sup>-</sup>, SH<sup>-</sup>, SeH<sup>-</sup>, an alkoxide of the formula R<sup>1</sup>O<sup>-</sup>, nitrate, a carboxylate of the formula R<sup>1</sup>COO<sup>-</sup>, cyclopentadienide (C<sub>5</sub>H<sub>5</sub><sup>-</sup>) or hydride (H<sup>-</sup>).

9. The process as claimed in one or more of claims 2, 4 and 5, characterized in that the iridium(III)-containing reactant contains a compound of the formula (V), (VII) and/or (VIII) and Y is the same or different at each instance and is H<sub>2</sub>O, H<sub>2</sub>S, a dialkyl sulfide of the formula (R<sup>1</sup>)<sub>2</sub>S, a thiol of the formula R<sup>1</sup>SH, an

alcohol of the formula  $R^1OH$ , an ether of the formula  $(R^1)_2O$ , a dialkyl sulfoxide  $(R^1)_2SO$ ,  $NH_3$ , a primary, secondary or tertiary amine, pyridine, quinoline, a nitrile of the formula  $R^1CN$ ,  $CO$ , a phosphine of the  
5 formula  $P(R^1)_3$ , a phosphine oxide of the formula  $OP(R^1)_3$ , an arsine of the formula  $As(R^1)_3$  or a phosphite of the formula  $P(OR^1)_3$ .

10. The process as claimed in one or more of claims 3,  
10 4, 5 and 6, characterized in that the iridium(III)-containing reactant is a compound of the formula (VI),  
(VII), (VIII) and/or (IX) and  $Z^0$  is the same or different at each instance and is bipyridine, phenanthroline, ethylenediamine, propylenediamine, or  
15 2-, 3- or 4-aminopyridine.

11. The process as claimed in one or more of claims 3,  
20 4, 5 and 6, characterized in that the iridium(III)-containing reactant is a compound of the formula (VI),  
(VII), (VIII) and/or (IX) and  $Z^1$  is the same or different at each instance and is diketonate, carboxylate, picolinate, aminocarboxylate, 1-ketoalkoxides, azide, cyanate, isocyanate, thiocyanate, isothiocyanate, chloride, bromide and iodide.

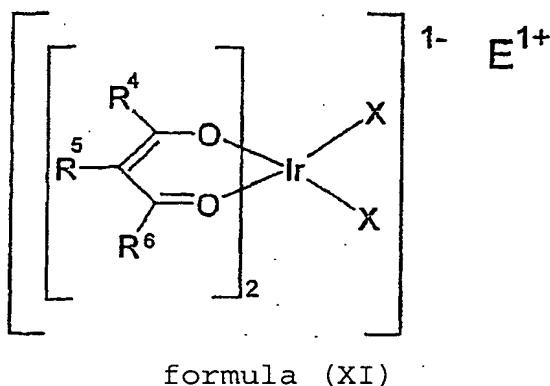
25 12. The process as claimed in one or more of claims 3,  
4, 5 and 6, characterized in that the iridium(III)-containing reactant is a compound of the formula (VI),  
(VII), (VIII) and/or (IX) and  $Z^1$  is the same or  
30 different at each instance and is acetylacetone or acetate.

13. The process as claimed in one or more of claims 3,  
35 4, 5 and 6, characterized in that the iridium(III)-containing reactant is a compound of the formula (VI),  
(VII), (VIII) and/or (IX) and  $Z^2$  is the same or different at each instance and is oxalate, malonate, phthalate, isophthalate, terephthalate, oxide or peroxide.

14. The process as claimed in claim 1 and/or claim 7, characterized in that the iridium(III)-containing reactant is a compound of the formula (X) in which Q is  
5 Cl, Br, I or a diketonate.

15. The process as claimed in claim 1 and/or claim 2, characterized in that the iridium(III)-containing reactant is a compound of the formula (V) in which X is  
10 the same or different at each instance and is a Cl, Br or I anion.

16. The process as claimed in one or more of claims 1, 2 and/or 15, characterized in that the iridium(III)-  
15 containing reactant contains a compound of the formula (XI)

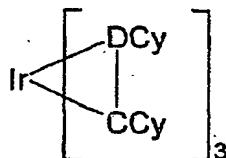


20 where R<sup>1</sup>, R<sup>2</sup>, R<sup>4</sup>, R<sup>5</sup> and R<sup>6</sup> are each as defined in claim 1, X is the same or different at each instance and is a Cl, Br or I anion, and E is an alkali metal cation, ammonium or phosphonium ion.

25 17. The process as claimed in one or more of claims 1 to 16, characterized in that the iridium(III)-containing reactant used contains a mixture of at least 2 iridium(III)-containing reactants of the formula  
30 (II), or (V) to (XI).

18. The process as claimed in one or more of claims 1 to 16, characterized in that the reactant used is a mixture which comprises at least one iridium(III)-containing reactant of the formula (II), or (V) to 5 (XI).

19. Homoleptic Ir(III) complexes of the formula (I)



10

formula (I)

in which:

CyD        is a cyclic group which contains at least one donor atom via which the cyclic group is bonded to the metal and which may in turn bear one or more substituents R; the CyD and CyC groups are joined together via a covalent bond;

CyC        is a cyclic group which contains a carbon via which the cyclic group is bonded to the metal and which may in turn bear one or more substituents R;

R            is the same or different at each instance and is F, Cl, Br, NO<sub>2</sub>, CN, a straight-chain or branched or cyclic alkyl or alkoxy group having from 1 to 20 carbon atoms, in which one or more nonadjacent CH<sub>2</sub> groups may be replaced by -O-, -S-, -NR<sup>1</sup>-, -CONR<sup>2</sup>-, -CO-O-, -CR<sup>1</sup>=CR<sup>1</sup>- or -C≡C-, and in which one or more hydrogen atoms may be replaced by F, or an aryl or heteroaryl group which has from 4 to 14 carbon atoms and may be substituted by one or more nonaromatic R radicals; where a plurality of substituents R, both on the same ring and on the two different rings, together

25

30

35

may in turn form a further mono- or polycyclic, aliphatic or aromatic ring system;

5           R<sup>1</sup> and R<sup>2</sup> are the same or different at each instance and are H or an aliphatic or aromatic hydrocarbon radical having from 1 to 20 carbon atoms,

10          characterized in that they have been obtained by a process as claimed in one or more of claims 1 to 18.

20. Homoleptic Ir(III) complexes as claimed in claim 19, characterized in that their purity is > 99%.